DEMONSTRATING DISCRETENESS AND COLLISION ERROR IN COSMOLOGICAL N-BODY SIMULATIONS OF DARK MATTER GRAVITATIONAL CLUSTERING

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ABSTRACT

Two-body scattering and other discreteness effects are unimportant in cosmological gravitational clustering in most scenarios, since the dark matter has a small particle mass. The collective field should determine evolution: Two–body scattering in simulations violates the Poisson–Vlasov equations. We test this in PM, P^3M, Tree, and NGPM codes, noting that a collisionless code will preserve the one–dimensional character of plane wave collapse. We find collisionality vanishing as the softening parameter approaches the mean interparticle separation. Solutions for the problem are suggested, involving greater computer power, PM–based nested grid codes, and a more conservative approach to resolution claims.

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1. Introduction

In the limit of small particle masses, a system of self–gravitating masses is described by the Poisson–Vlasov equations: the particle–particle scattering becomes unimportant, and the evolution approaches that of a continuous system with a time–dependent potential (Chandrasekhar 1942; Sellwood 1987). N-body codes have a small number of high mass particles compared to a Universe of unclustered dark matter. It is not clear whether the ensemble converges to some or all of the properties of the right solution (Melott 1981). In fact, one may conclude that if "...much of the mass in the universe comprises an invisible component (the missing mass) there is no guarantee that the galaxies have ever acted as point particles. If this were the case, the results from N–body experiments would not apply to the real universe." (Hockney and Eastwood 1981, 1988). The purpose of the Letter is to present preliminary results from a longer study to warn of possible problems.

The mean–field approach is typified by the particle–mesh, or PM method (Doroshkevich et. al 1980; Melott 1981, 1982b; Klypin & Shandarin 1983). Particles move in a gravitational potential computed on a mesh. The shortcoming is that there are no valid results below the mesh scale, since potential and density are smoothed over that scale. So far no errors have been reported other than this (rather serious) limitation.

Short–range forces may be added to preserve the r^{-2} force law in close encounters. P^3M (Particle–Particle–Particle Mesh) (Hockney & Eastwood 1981; Efstathiou & Eastwood 1981) and Tree codes (Suginohara et al. 1991) are two examples, although more recently codes based on adaptive mesh refinement (Pen 1995; Suisalu & Saar 1995; Gelato et al. 1996; Kravtsov et al. 1996), have been used. Generally this approach improves resolution of the Green function for the Poisson equation without improving the resolution of the source term. For this reason we call them HFLMR (High Force Low Mass Resolution) codes. Roughly isotropic contraction of clumps is often used to justify this approach. Tests made

by Kuhlman et al. (1996) on generic smooth initial perturbations do not support isotropic collapse. To prevent the formation of tight binaries which slow down execution, all codes resort to force softening, so that on scales less than ϵ the force law is softer than $1/r^2$. Values of ϵ (in units of the mean interparticle separation $n^{-1/3}$) of 0.01 to 0.2 are common and results are usually presented down to ϵ. We will show that $\epsilon \sim 1$ is needed to maintain a collisionless, quasi–continuous system.

Computer codes are often cross-checked for convergence, but a common assumption may lead to a common error. Agreement with exact solutions is better, but not easy. One classic test for two–body scattering error is mass segregation. Particles of higher mass settle to inner parts of bound systems due to equipartition proceeding by two–body scattering. Efstathiou & Eastwood (1981) found strong segregation in $\mathrm{P^3M}$. This result appears to have been largely ignored. Peebles et al (1989) verified that it could be suppressed in PM with $\epsilon \sim 1$. In an equal mass system, like most cosmological simulations, this error may exist but not result in segregation. Suisalu & Saar (1996) examined deflections and found an indication of trouble in a $\mathrm{P^3M}$ code, but their original method was unable to show whether the scattering was due to mean field or two-body fluctuations.

2. Plane–Symmetric Collapse

We suggest a new type of test (symmetry-breaking) for codes in the nonlinear regime without an exact solution. We use a simple system with a clear prediction: plane–wave collapse. (Of course it could be spherical collapse, two-dimensional collapse onto a filament, or any other type of symmetric collapse.) This has an exact solution up to shell crossing (Zel'dovich 1970; Shandarin & Zel'dovich 1989), and was used by Efstathiou et al. (1985) in code testing. However, they worked only in the precollapse regime and along coordinate axes so no collisions were possible. Obviously a collisionless system with only one–dimensional

perturbations should remain one-dimensional. This is the basis of our test, violation of which means the code is collisional or otherwise erroneously scattering particle orbits.

We make the test more relevant by tilting the plane of collapse relative to the simulation cube. We set up a single perturbation wave $\mathbf{k} = (2,3,5)k_f$ ($|\mathbf{k}| = 6.16k_f$, where k_f is the fundamental mode) by Fourier transform on a grid of 64^3 particles. We began with an amplitude $\delta \equiv (\rho - \bar{\rho})/\bar{\rho} \sim 0.1$, and evolved for an expansion factor of 7.7 after the first shell crossing, during which collisions can happen. While the physical system should have no scattering, near misses may generate them numerically. The role of the symmetry is only to make it detectable. To perform the comparison we used a PM (Melott 1981, 1986), a P^3M (kindly supplied by H. Couchman 1991) and a Tree-code (Suginohara et al. 1991). We also tested the Nested–Grid Particle–Mesh (NGPM) code (Splinter 1996). All runs had identical (publicly available) initial conditions. The initial conditions for the NGPM code were generated in the above manner for both the coarse and fine grid. We also did cross check runs in which the perturbation $\mathbf{k} = (0, 0, 6)k_f$ was *not* tilted with respect to the cube.

The PM run was performed on a 64^3 mesh and duplicated on a 128^3 mesh to emulate a sometimes used modification as well as verify the code-independence of our results. PM tests were done with traditional two-point differencing and the Melott (1986) improved force resolution staggered mesh scheme. There was no significant difference in scattering and we report the latter here. We performed otherwise identical P^3M and Tree tolerance parameter $\theta = 0.2$ runs with $\epsilon = 0.1$, and 1.0, plus a transitional P^3M run with $\epsilon = 0.5$. In the P^3M code, we used two choices of time integration variable and varied the timestep greatly, assuring satisfaction of both Courant and leapfrog stability conditions. The PM and NGPM codes automatically test and adjust timesteps as needed. The adaptive smoothing length capability of the P^3M code was turned off as suggested by Gelb and Bertschinger (1994). The NGPM code had a refinement factor of 8, putting it close in spatial resolution

to the $\epsilon = 0.1$ P^{3}M run, but with 512 times increased mass resolution (an "HFHMR" code). Results of a much more extended study will be presented elsewhere.

Figure 1 shows the overall configuration of the PM system after collapse. All runs look roughly similar. Differences between tilted runs are shown in Figure 2, in which slices of one collapsed planar region are projected along initial perturbation axis. The only inhomogeneity should be projection of the initial lattice onto this plane. Some runs show clumping, suggesting scattering error. What all the erroneous HFLMR runs (the P^{3}M and Tree code runs with $\epsilon < 1$, and the 128^3 mesh PM run) share are softening lengths shorter than the mean interparticle separation. The runs that performed well (normal PM, P^{3}M and Tree with $\epsilon = 1$, and NGPM) all have softening comparable to this distance; of course for NGPM this is a considerably smaller distance, but at no collision penalty. (Axis–aligned PM and P^{3}M runs show the lattice, with no clumping visible.)

We use as one quantitative measure the distribution of particle velocities. They should be strictly normal to the planes; we separate them into components along the normal and in the plane $V_{plane} = \sqrt{V_{p1}^2 + V_{p2}^2}$. Figure 3 shows scatter plots for 1000 randomly selected particles from each of our runs. Many are hidden by superposition. The correct result is a line along the V_{norm} axis. This is approached only by non–sparse PM and NGPM, by P^{3}M and Tree as the short–range force is turned off, and by axis–aligned runs which have only head–on collisions. With $\epsilon = 0.1$, the most common choice, the error is large.

The relative error can be made quantitative by comparing the median speed in the plane to the median speed along the normal, as shown in Table 1. Another measure is the kinetic energy; the mean from motion in the plane and along the normal are also shown in Table 1. Lastly, we show the median value of d_{plane}, the distance in mesh units particles have strayed off the normal trajectory. All values are the mean or median of 10,000 particles (subgrid particles in NGPM). Our axis–aligned PM and P^{3}M runs had *zero* off–normal

velocity (within computer precision).

Figure 4 shows a phase–space diagram of a single sheet, including the normal displacement and velocity, with the other four phase space dimensions suppressed. The correct solution is a well–known spiral (Doroshkevich et al. 1980; Melott 1982a; Bond et al. 1983). The codes that preserve this pattern are those with softening comparable to the mean interparticle separation.

We can verify that scattering is from encounters and not the initial gravity fields by noting that off-normal components are small until shell crossing in all codes; they increase strongly in the inclined HFLMR codes as particles pass each other.

3. Discussion

We have shown that HFLMR computational methods in widespread use for gravitational clustering in cosmology perform incorrectly on a simple test problem, as a consequence of trying to model a continuous system with discrete masses. The PM and NGPM methods (as normally used) are able to handle this test because there is no evasion of the discreteness limitation. PM can be forced to fail by increasing the lattice resolution beyond appropriate limits. HFLMR methods work properly if the short range force is turned off or if they are forced to alignment with the coordinate axes.

As convergence to the proper behavior is very slow (e.g. Hockney, 1971), past comparisons by varying particle number have not revealed this (e.g. Efstathiou & Eastwood 1981). Coupling these incorrectly evolved systems to hydrodynamics will guarantee that it is being done in the wrong background gravitational potential. We do not claim the effect will move to larger scales. Melott and Shandarin (1990), Little et al. (1991), and Melott & Shandarin (1993) have shown that small scale effects scarcely propagate to large scales, but

more quantitative study is needed. However, errors would only stop growing in voids or in regions where the particle density exceeds ϵ^{-3}.

Questions may be raised about the relevance of our example. Galaxies are not infinite planes. However, the first collapse on any scale is expected to be sheet–like (Shandarin et al. 1995; Kuhlman, et al. 1996; Gouda 1996) so there is ample opportunity for this situation to arise. Furthermore, collisionality operates in the absence of symmetry; our planar collapse study simply makes it starkly obvious. One may argue that since collapsed pancakes are unstable to small–scale perturbations, the HFLMR codes model this correctly, justifying the results they give for small ϵ. Since there is no small-scale power in the initial conditions, these codes are artificially producing power on small–scales by the growth of shot noise. The results of a simulation should be a consequence of initial conditions that were imposed. This is illustrated in the orientation-dependence of the HFLMR codes: Since we get two completely different results depending on orientation, one must ask, "Which is correct?" Most importantly, this serves to raise the question of whether a code performs well overall in a complex nonlinear problem when it cannot replicate a simple test case. As this Letter was going to press, we learned of Park (1997), in which spherical collapse is studied, producing conclusions close to ours. Values $\epsilon = 0.01$ or even smaller are used in clustering studies.

One might hope that realistic cosmological scenarios with power on all scales avoid this problem. Impressed perturbations might overwhelm discreteness if the spectrum is normalized to the shot noise level at the particle Nyquist frequency (Efstathiou et al. 1985). We tested this by putting in an inclined plane wave close to the particle Nyquist frequency, at the white noise amplitude. Again we found strong scattering in a $\epsilon = 0.1$ P^{3}M run, and essentially none in PM. At this short wavelength the resolution limitations of PM show themselves in its lower velocity dispersion, so both codes are performing badly. The

accuracy of cosmological results from HFLMR codes remains an open question.

Suto (1991) examined the divergence of particle trajectories in a series of N–body cosmological simulations varying ϵ. He found that the comoving trajectories diverged with time as $e^{\lambda t}$, fitting $\lambda \simeq 0.05\sqrt{G\bar{\rho}}\epsilon^{-1.2}$. By requiring $e^{\lambda t_H} < \epsilon$, where t_H is the Hubble time we require that deflection of nearby trajectories by shot noise is small. Enforcing such a condition gives $\epsilon \gtrsim 1$, similar to our results, the results of Peebles et al. (1989) and Suisalu and Saar (1996).

One promising method to achieve better force and mass resolution while doing correct physics is nested–grid methods, which put more particles in a region of interest. Such methods are shown here to greatly reduce collisions and may allow the study of small–scale structure to progress (e.g. Villumsen 1988; Anninos et al. 1994; Splinter 1996). Putting in a higher particle density acknowledges the inability get something for nothing by sidestepping the laws of physics.

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REFERENCES

Anninos, P., Norman, M., & Clarke, D.A. 1994 ApJ, 436, 11

Bond, J.R., Szalay, A., & White, S.D.M. 1983 Nature 301, 584.

Chandrasekhar, S. 1942 Principles of Stellar Dynamics, (New York: Dover Publications)

Couchman, H. 1991 ApJ, 368, L23

Doroshkevich, A.G., Kotok, E.V., Novikov, I.D., Polyudov, A.N., Shandarin, S.F., & Sigov, Yu.S. 1980 MNRAS, 192, 321.

Efstathiou, G.E., Davis, M., Frenk, C.S. & White, S.D.M. 1985 ApJS, 57, 241

Efstathiou, G.E. & Eastwood, J.W. 1981 MNRAS, 194, 503

Gelato, S., Chernoff, D.F. & Wasserman, I. 1996 ApJ submitted, astro-ph/9607156

Gelb, J.M., & Bertschinger, E. 1994 ApJ, 436, 467

Gouda, N. 1996, preprint

Hockney, R.W. 1971 J Comp Phys, 8, 19

Hockney, R.W. & Eastwood, J.W. 1981,1988 Computer Simulation Using Particles (New York: McGraw-Hall), p. 454

Kravtsov, A.V., Klypin, A.A., & Khokhlov, A.M. 1996 preprint.

Kuhlman, B., Melott, A.L., & Shandarin, S.F. 1996 ApJL, 470, L1

Klypin, A.A. & Shandarin, S.F. 1983 MNRAS, 204, 891

Little, B., Weinberg, D.H., & Park, C. 1991 MNRAS, 253, 295.

Melott, A.L. 1981 Ph.D. Thesis, University of Texas

Melott, A.L. 1982a Phys.Rev.Lett. 51, 935.

Melott, A.L. 1982b Nature, 296, 721

Melott, A.L. 1986 Phys Rev Lett, 56, 1992

Melott, A.L. & Shandarin, S.F. 1990 Nature 346, 633

Melott, A.L. & Shandarin, S.F. 1993 ApJ, 410, 469

Park, C.B. 1997 AAS Poster presentation.

Peebles, P.J.E., Melott, A.L., Holmes, M.R., Jiang, L.R., 1989 ApJ, 345, 108

Pen, Ue-Li 1995 ApJS, 100, 269

Sellwood, J.A. 1987 ARAA, 25, 151

Shandarin, S.F., McDavitt, K., Pauls, J.L, & Tinker, J. 1995 Phys Rev Lett, 75, 7

Shandarin, S.F., & Zel'dovich, Ya.B. 1989 Rev Mod Phys, 61, 185

Splinter, R.J. 1996 MNRAS, 281, 281

Suisalu, I. & Saar, E. 1995 MNRAS, 274, 287

Suisalu, I. & Saar, E. 1996 MNRAS, submitted astro-ph/9511120

Suginohara, T., Suto, Y., Bouchet, F.R., & Hernquist, L. 1991 ApJS, 75, 631

Suto, Y. 1991 Publ Astron Soc Japan, 43, L9

Villumsen, J.V. 1988 ApJS, 71, 407

Zel'dovich, Ya.B. 1970 AA, 5, 84

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Fig. 1.— The configuration of particles at the end of our PM simulation. The other simulations look much the same except for more inhomogeneity in some cases.

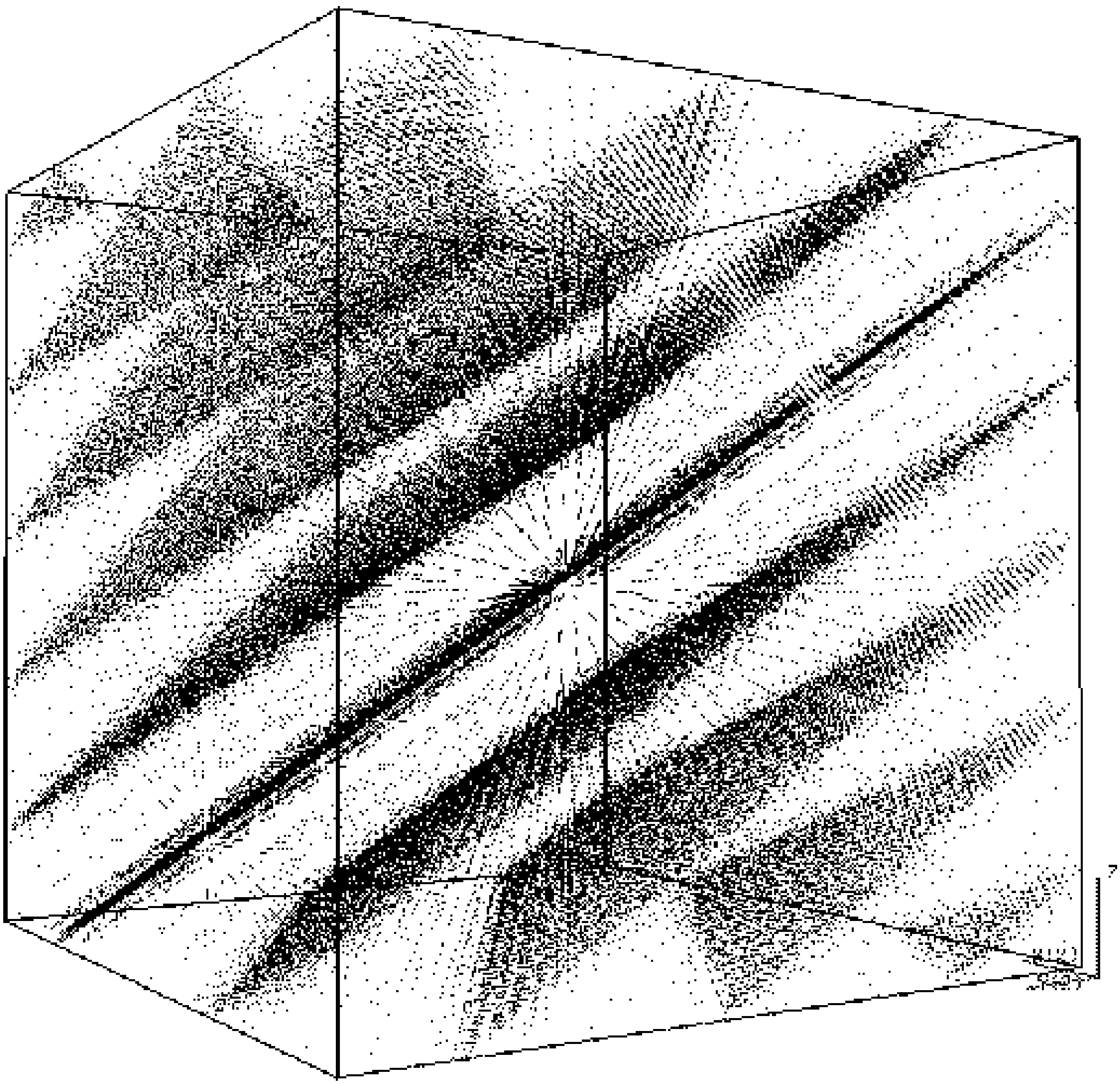
Fig. 2.— A slice of one of the planes from each cube, seen projected along the normal to the plane. The dimensions of the slice are $16 \times 16 \times 4$. To construct the NGPM slice a slice of size $4 \times 4 \times 1$ was extracted from the sub–grid particles and repeated periodically to produce a slice of size $16 \times 16 \times 4$. This slice was then sampled to reduce the number of particles to roughly that of the other runs. The arrangement of panels is: Top row–PM with one particle per cell, PM with one particle per 8 cells (a common 'resolution increasing' procedure) and NGPM (Sub–grid). Middle row–P^3M with specified value of ϵ. Bottom row–Tree code with the specified ϵ, and the correct result, which was constructed by propogating particles along normals to the plane; the appearance of lines is a tilted projection of the cubic lattice. This projection represents the standard for all except NGPM, which shows correct appearance.

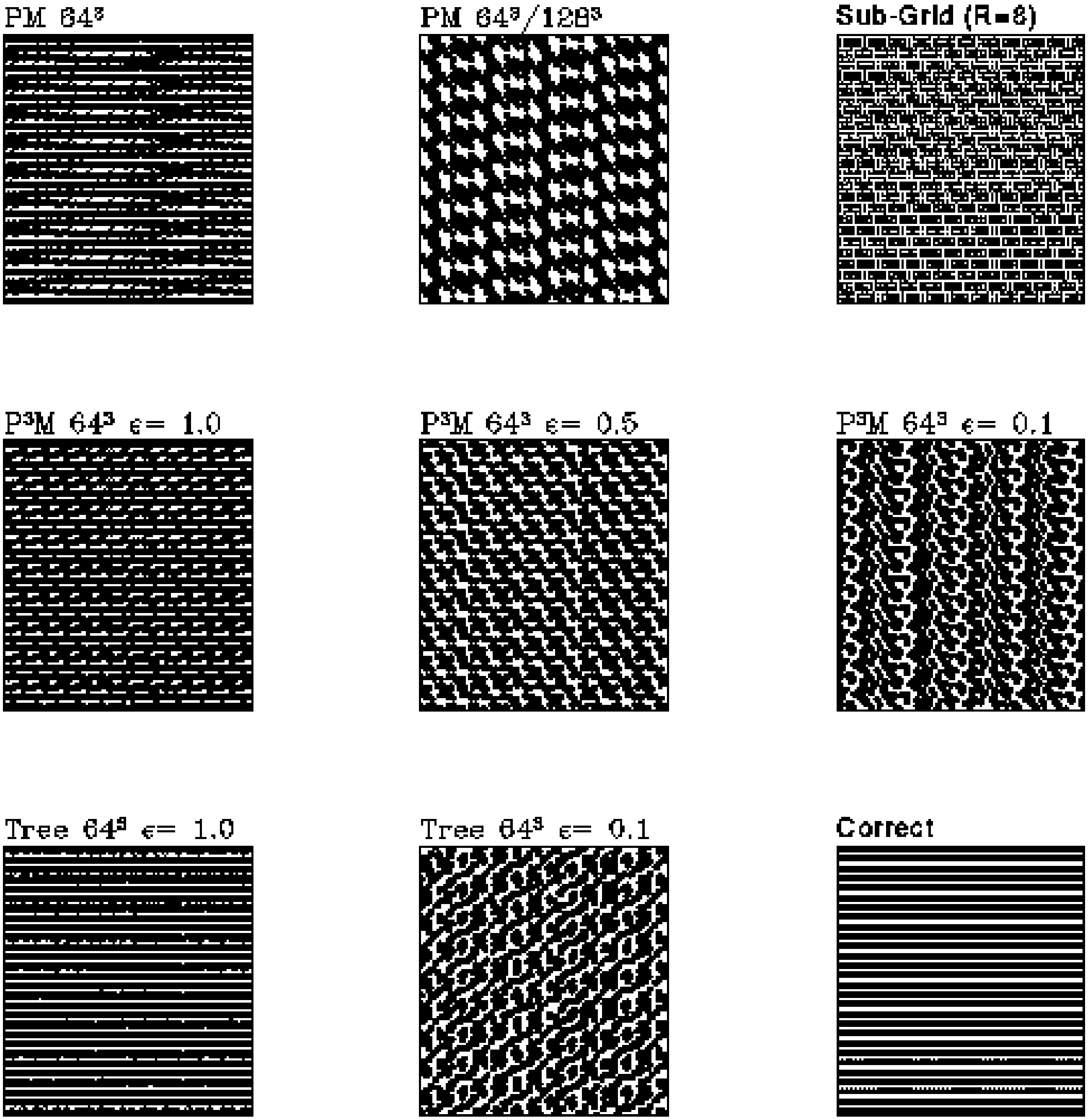
Fig. 3.— Scatter plots of the absolute value of velocity components for 1000 particles randomly selected from each of the simulations, projected along the normal to the plane of collapse, and in that plane. For correct physical modeling, all points should lie along the x axis. Each plot contains the same number of points; many are superimposed. Same arrangement as Fig. 2. Velocity units are Hubble velocity across one cell.

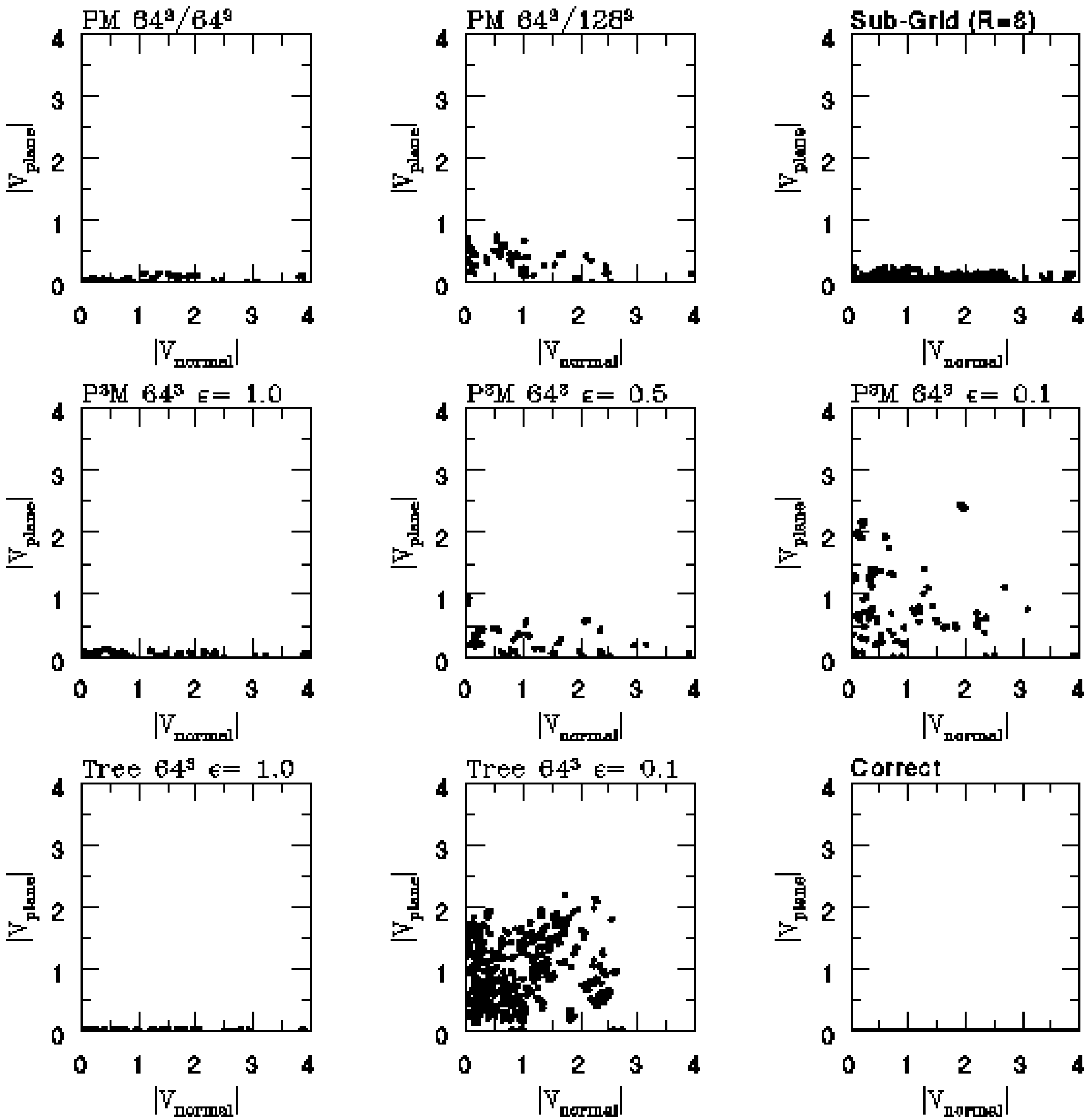
Fig. 4.— Scatter plots of the normal component of the velocity for all particles collapsed toward one of the pancake planes, against their displacement from the midpoint. The known solution is a sprial pattern, whose development varies with resolution in some codes, but is totally disrupted in others. Same arrangement and units as in Fig. 3.

Table 1. Code Comparison–Plane Wave Test

Code	$med(V_{norm})$	$med(V_{plane})$	$\bar{T}_{norm}$	$\bar{T}_{plane}$	$med(d_{plane})$
PM	0.75	0.03	1.82	0.001	0.01
PM($N_c = 128^3$,$N_p = 64^3$)	0.91	0.44	2.53	0.22	0.80
Sub-Grid(R=8)	0.77	0.05	1.84	0.02	0.003
$P^3M(\epsilon = 1.0)$	0.70	0.05	1.99	0.004	0.03
$P^3M(\epsilon = 0.5)$	0.82	0.27	2.00	0.15	0.12
$P^3M(\epsilon = 0.1)$	0.78	0.62	2.10	0.76	0.53
Tree($\epsilon = 1.0, \theta = 0.2$)	0.57	0.01	1.82	0.0003	0.02
Tree($\epsilon = 0.1, \theta = 0.2$)	0.81	0.62	2.08	0.79	0.45




PM 64^3
PM $64^3/128^3$
Sub-Grid (R=8)
P^{3}M 64^3 ϵ= 1.0
P^{3}M 64^3 ϵ= 0.5
P^{3}M 64^3 ϵ= 0.1
Tree 64^3 ϵ= 1.0
Tree 64^3 ϵ= 0.1
Correct


PM 64³/64³
PM 64³/128³
Sub-Grid (R=8)
P³M 64³ ε= 1.0
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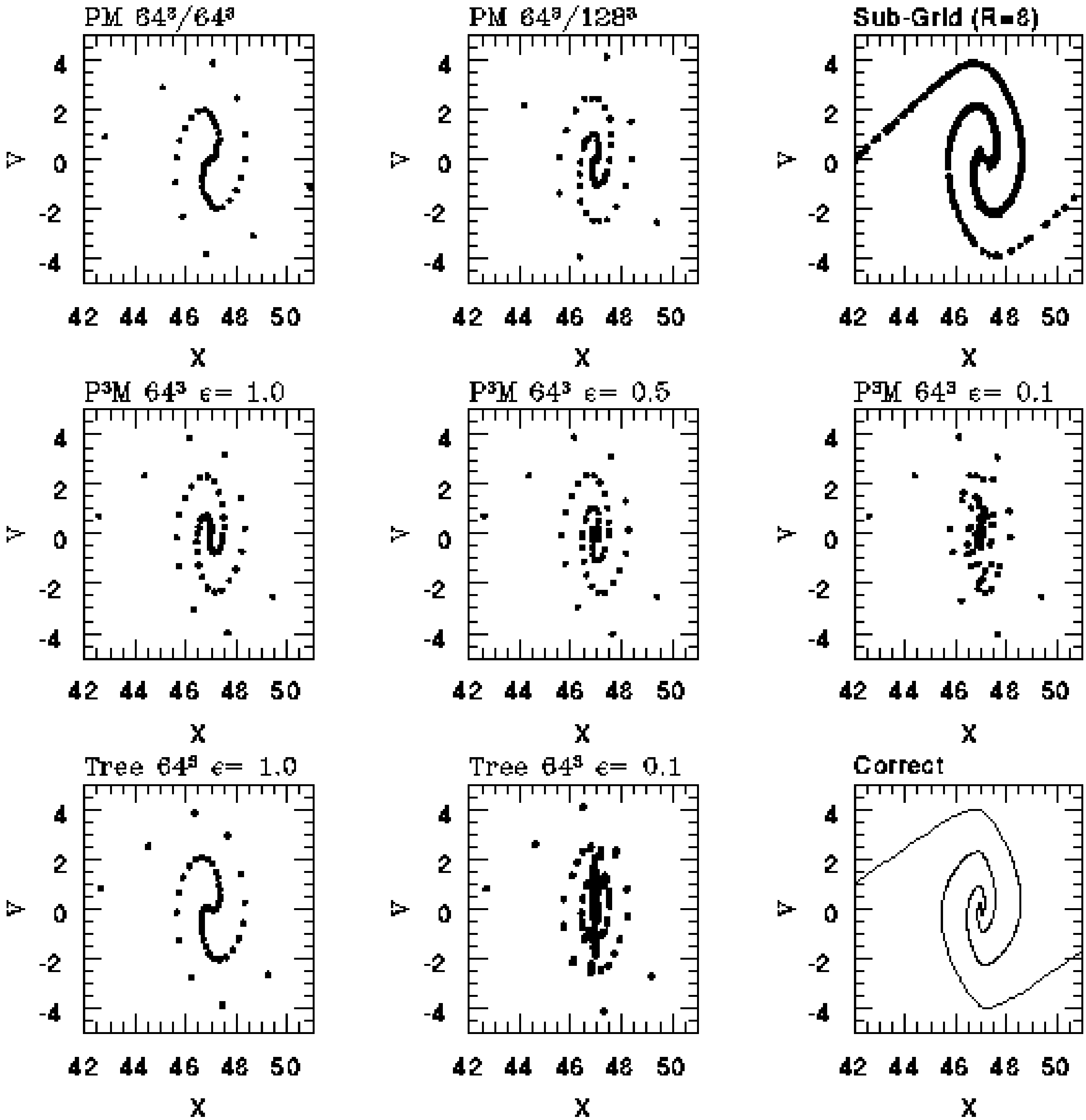
Correct
|V_plane|
|V_normal|


PM $64^3/64^3$
PM $64^3/128^3$
Sub-Grid (R=8)
P^3M 64^3 ϵ= 1.0
P^3M 64^3 ϵ= 0.5
P^3M 64^3 ϵ= 0.1
Tree 64^3 ϵ= 1.0
Tree 64^3 ϵ= 0.1
Correct
X
V